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DETERMINATION OF OXYGEN AND CARBON IN SILICON WAFERS  
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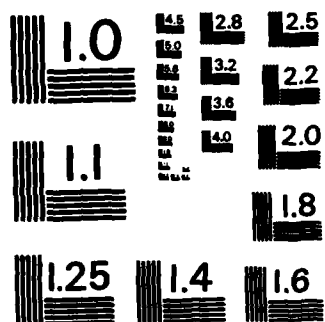
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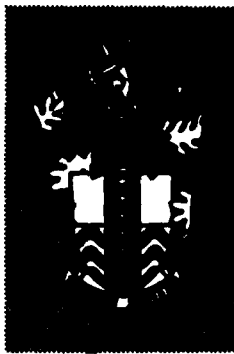


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**RSRE  
MEMORANDUM No. 3479**

**ROYAL SIGNALS & RADAR  
ESTABLISHMENT**

**DETERMINATION OF OXYGEN AND CARBON IN SILICON WAFERS**

**Author: R W Series**

**PROCUREMENT EXECUTIVE,  
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# ROYAL SIGNALS AND RADAR ESTABLISHMENT

Memorandum 3479

Title: DETERMINATION OF OXYGEN AND CARBON IN SILICON WAFERS  
 Author: R W Series  
 Date: August 1982

## SUMMARY

Possibilities for the use of a dispersive infrared spectrophotometer to determine the oxygen and carbon content of device quality silicon wafers have been examined. A novel approach to the analysis of the spectra based on a curve fitting method has been employed. This has been shown to provide very good rejection of interferences due to absorptions caused by precipitates present in heat treated material. Single instrument precisions for measurements on 350 $\mu$ m device quality wafers of better than 10% for oxygen and  $\pm 2 \times 10^{16}$  atom cm<sup>-3</sup> for carbon with no correction for wafer backsurface finish are reported.

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DETERMINATION OF OXYGEN AND CARBON IN SILICON WAFERS

R W Series

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1 INTRODUCTION

This memorandum summarises results of a study conducted at RSRE into development of methods suitable to determine the oxygen and carbon content of device quality silicon wafers using measurements based on local mode infrared absorption at  $1106\text{ cm}^{-1}$  and  $605\text{ cm}^{-1}$ . The equipment consists of a Perkin Elmer 580B dispersive ratio recording infrared spectrophotometer and a model 3500 data station. All computing was carried out using standard BASIC as supplied with the data station. The emphasis of the work has been to develop quick, non destructive methods which are as insensitive as possible to surface finish and other interferences. In keeping with these constraints no attempt has been made to use low temperature measurements or special sample preparation techniques. Two differing mathematical methods have been used to analyse the spectra. The first is based on integrated area measurements and the second on a curve fitting method developed at RSRE. While there is little to chose between the two, the curve fitting method offers improved performance for difficult and heat treated samples. The method has been routinely used at RSRE for over a year with no problems.

Copies of the program, which include provision for fully automatic control of the spectrophotometer are available on request.

## 2 CONVERSION OF TRANSMITTANCE TO ABSORBANCE

When using any analytic method to analyse the spectra it is necessary first to convert the measured transmittance to absorbance. As shown in reference 1 the approximations commonly used may lead to errors in excess of 15% when thin wafers are measured. The effects of various approximations for the conversion of transmittance to absorbance have therefore been examined.

The transmission through a sample with both surfaces polished may be written (neglecting interference effects);

$$T = (1-R)^2 \exp(-a) / (1-R^2 \exp(-2a)) \quad (2.1)$$

where R is the reflection coefficient and a the absorbance.

To a first approximation

$$a = -\ln(T) + 2\ln(1-R) \quad (2.2)$$

which is the most commonly used relationship. A much better approximate solution is

$$a = -\ln(T) - \ln\left(\frac{(1-R^2)}{(1-R)^2}\right) + R^2 (1-T^2) \left(\frac{(1-R^2)}{(1-R)^2}\right)^2 \quad (2.3)$$

With this approximation the errors are less than 4% for all values of a.

With samples in both reference and sample beams the corresponding equations are

$$\beta - a = -\ln(T) \quad (2.4)$$

$$\beta - a = -\ln(T) + R^2 \exp(-2\beta) (T^2 - 1) \quad (2.5)$$

where  $\beta$  is the absorbance in the reference beam.

Physically the difference between the approximations corresponds to the difference between light passing once through the sample, and account being made of multiple reflections within the sample (fig 1).



FIGURE 1

For well polished samples approximation 2-3 and 2-5 are to be preferred, but for wafers with heavy back surface damage it is possible that reflection at the rough surface is suppressed such that 2-2 and 2-4 provide better descriptions. This point can only be resolved by experiment as discussed later.

### 3 INTEGRATED AREA MEASUREMENT METHOD

The spectra are scanned and converted to absorbance. Linear baselines are fitted to the oxygen band and the carbon/silicon band. The integrated areas in the range  $1120-1090\text{ cm}^{-1}$  for the oxygen band,  $630-610\text{ cm}^{-1}$  for the lattice absorption,  $610-595\text{ cm}^{-1}$  for the carbon absorption are then used to compute thickness, oxygen and carbon difference between the sample and reference.

$X_1$  = integrated area  $1120-1090\text{ cm}^{-1}$  (corrected for baseline)

$X_2$  = integrated area  $630-610\text{ cm}^{-1}$  (corrected for baseline)

$X_3$  = integrated area  $610-595\text{ cm}^{-1}$  (corrected for baseline)

$$X_1 = C_0 \Delta T + C_1 (T - \Delta T) [O] \quad (3.1)$$

$$X_2 = C_2 \Delta T + C_3 (T - \Delta T) [C] \quad (3.2)$$

$$X_3 = C_4 \Delta T + C_5 (T - \Delta T) [C] \quad (3.2)$$

where  $C_0$  = Si matrix absorption per unit thickness over oxygen band.

$C_1$  = Oxygen absorption for unit oxygen content.

$C_2$  = Si matrix absorption per unit thickness over  $630/610\text{ cm}^{-1}$  band

$C_3$  = Carbon absorption per unit concentration over  $630/610\text{ cm}^{-1}$  band

$C_4$  = Si matrix absorption per unit thickness over  $610/595\text{ cm}^{-1}$  band

- $C_3$  = Carbon absorption per unit concentration over 610/595  $\text{cm}^{-1}$  band
- $T$  = Thickness of reference sample
- $\Delta T$  = Thickness difference between reference and sample
- $|O|$  = Oxygen concentration of sample
- $|C|$  = Carbon concentration of sample

Note:- the reference is assumed to have negligible carbon and oxygen.

Constants  $C_0$ - $C_3$  are obtained using standards with known oxygen and carbon content. The results described later used two standards, one 1.91 mm thick and containing no detectable oxygen or carbon and one 1.905 mm thick containing  $7.7 \times 10^{16}$  atom  $\text{cm}^{-3}$  carbon and  $0.92 \times 10^{18}$  atom  $\text{cm}^{-3}$  oxygen (old ASTM calibration). Scans were made of the pure standard using air as a reference and then of the impure standard using the pure standard as a reference. Using this data equations 3.1, 3.2 and 3.3 were solved for  $C_0$ - $C_3$ .

To determine the oxygen and carbon content and thickness of unknown samples equations 3.2 and 3.3 were solved for  $\Delta T$  and  $|C|$ . Equation 3.1 was then solved for  $|O|$ . This avoids the necessity of measuring the sample thickness by a separate technique. An incidental advantage is that if equation 2.2 or 2.4 is used to convert transmittance to absorbance the errors introduced by the approximations involved tend to cancel each other when the oxygen or carbon concentrations are evaluated. That is the thickness estimates tend to show more error than either the oxygen or carbon content.

#### 4 CURVE FITTING METHOD

The IR spectrum is scanned 1200-1000  $\text{cm}^{-1}$  and 640-500  $\text{cm}^{-1}$  (or as required). The 640/500 band data is processed to give the thickness and carbon content. The 1200/1000  $\text{cm}^{-1}$  band spectra is then used to determine the oxygen content. Linear baselines (in absorbance) are assumed for both bands. All calculations are performed in absorbance units.

##### 4.1 Analysis

For the oxygen peak

$$A_1(x_1) = a_0 + a_1 x_1 + a_2 f_{11}(x_1) + a_3 f_{12}(x_1) + \delta_1 \quad (4.1)$$

and for the carbon peak



$$A_i(x_i) = a_4 + a_5 x_i + a_2 F_{21}(x_i) + a_6 F_{22}(x_i) + \delta_i \quad (4.2)$$

where

$A_i(x_i)$  • absorbance difference between sample and reference

$x_i$  • Wavenumber - effect

$\left. \begin{matrix} a_0 \\ a_1 \end{matrix} \right\}$  • linear baseline terms

$a_2$  • Difference in thickness between sample and reference

$a_3$  • Oxygen in sample - oxygen in reference

$\left. \begin{matrix} a_4 \\ a_5 \end{matrix} \right\}$  • Linear baseline terms

$a_6$  • Carbon in sample - Carbon in reference

$F_{11}$  • Silicon absorption over oxygen band

$F_{12}$  • Oxygen absorption

$F_{21}$  • Silicon absorption over carbon band

$F_{22}$  • Carbon absorption over carbon band

$\delta_i$  • random noise

The wavenumber effect is chosen to give the origin at the mid-point of each band. For a least squares fit we wish to minimize

$$\sum (A_i(x_i) - a_0 - a_1 x_i - a_2 F_{11}(x_i) - a_3 F_{12}(x_i))^2 \quad (4.3)$$

with respect to  $a_0$ ,  $a_1$  and  $a_3$  and also

$$\sum (A_i(x_i) - a_4 - a_5 x_i - a_2 F_{21}(x_i) - a_6 F_{22}(x_i))^2 \quad (4.4)$$

with respect to  $a_2$ ,  $a_4$ ,  $a_5$ ,  $a_6$ . Note that only the 640/300  $\text{cm}^{-1}$  band data is used to obtain the thickness estimate. This is because the 640/300  $\text{cm}^{-1}$  band is most strongly dependent on the thickness of the sample and changes in the shape of the oxygen peak due to heat treatment etc might cause spurious results if the 1200/1000  $\text{cm}^{-1}$  band data were included in the estimation of  $a_2$ .

As shown in section 4.2,  $F_{jk}(x_i)$  has the property

$$\sum_i P_{jk}(x_i) = 0 \quad (4.5)$$

$$\sum_i x_i P_{jk}(x_i) = 0 \quad (4.6)$$

Minimization of 4.3 and 4.4 then gives:

$$a_2 = (S_1 S_2 - S_3 S_4) / (S_3 S_2 - S_4^2) \quad (4.7)$$

$$a_6 = (S_1 S_4 - S_3 S_5) / (S_4^2 - S_5 S_6) \quad (4.8)$$

$$a_7 = (S_7 - a_2 S_8) / S_9 \quad (4.9)$$

where

$$S_1 = \sum P_{21}(a_1) \cdot A_2(a_1)$$

$$S_2 = \sum P_{22}(a_1)^2$$

$$S_3 = \sum P_{22}(a_1) \cdot A_2(a_1)$$

$$S_4 = \sum P_{21}(a_1) \cdot P_{22}(a_1)$$

$$S_5 = \sum P_{21}(a_1)^2$$

$$S_7 = \sum A_1(a_1) \cdot P_{12}(a_1)$$

$$S_8 = \sum P_{11}(a_1) \cdot P_{12}(a_1)$$

$$S_9 = \sum P_{12}(a_1)^2$$

Knowing the thickness, oxygen and carbon content of the reference the thickness, oxygen and carbon content of the sample may now be found.

## 4.2 Creation of Equations

Two standard samples are used. Spectra are recorded of one using an air reference, then the difference spectra are measured. Conditions should be chosen so that the spectra may be treated as noise free.

$$A_1(a_1) = b_0 + b_1 a_1 = b_0 P_{11}(a_1) + b_9 P_{12}(a_1) \quad (4.10)$$

$$A_2(a_1) = b_2 + b_3 a_1 = b_8 P_{21}(a_1) + b_{10} P_{22}(a_1) \quad (4.11)$$

$$A_3(a_1) = b_4 + b_5 a_1 = b_{11} P_{11}(a_1) + b_{12} P_{12}(a_1) \quad (4.12)$$

$$A_4(a_1) = b_6 + b_7 a_1 = b_{11} P_{21}(a_1) + b_{13} P_{22}(a_1) \quad (4.13)$$

where  $a_0 = b_0$  are baseline terms

$b_0$  is the thickness of standard 1

$b_0$  is the oxygen content of standard 1

$b_{10}$  is the carbon content of standard 1

$b_{11}$  is the thickness difference between standards 1 and 2

$b_{12}$  is the oxygen difference between standards 1 and 2

$b_{13}$  is the carbon difference between standards 1 and 2

$S_j(x_i)$  are the spectra in absorbance units.

To fix the baseline terms rather than pick arbitrary values for  $b_0 = b_1$  we instead define the baselines such that

$$\sum_k F_{1j}(x_k) = 0 \quad (4.14)$$

$$\sum_k x_k F_{1j}(x_k) = 0 \quad (4.15)$$

Equations 4.14 to 4.15 can be solved for  $F_{1j}(x_k)$ .

## 5. RESULTS

The performance of both methods depends on the accuracy with which the calibration is carried out and instrument conditions used. It has been found that the most satisfactory procedure is to use two standards, well matched in thickness and one containing a high level of carbon and oxygen. Our normal method is to use one reference standard 1.710 cm thick with no detectable carbon or oxygen and one standard 1.905 cm thick and containing  $0.91 \pm 10^{18}$  atoms  $\text{cm}^{-2}$  oxygen and  $1.1 \pm 10^{18}$  atoms  $\text{cm}^{-2}$  carbon (as determined using the old ASTM method). First the reference is scanned against air, then the C2 standard is scanned against the reference. This procedure minimizes errors introduced by instrument drift etc.

With suitable instrumental conditions (see below), when using the curve fitting method and using constantly 2 cm cell polished samples oxygen measurements are reproducible to better than  $\pm 3\%$  and carbon to  $\pm 10\% \pm 2 \times 10^{15}$  atoms  $\text{cm}^{-2}$ . For 100 um device quality wafers, where an air reference method is used errors are about  $\pm 10\%$  for oxygen and  $\pm 2 \times 10^{16}$  atoms  $\text{cm}^{-2}$  for carbon. Total time for measurement and calculation is about 8 mins if both carbon and oxygen analysis is required or 3 mins if only the oxygen content is required.

### 5.1 Effect of Slit Width

Theories for the integrated area measurement and also the curve fitting method both rely on the assumption that Beers law applies. Beers law may fail for a number of reasons. One of the most common causes is that the finite slit width may cause broadening of the peaks. Although, in the case of a single peak it is possible to construct a calibration curve and so correct for deviations from Beers law, this is not possible in the case of overlapping bands. Tests were therefore carried out to determine at what resolution departures from Beers law linearity became a problem. Difference spectra were recorded from five samples nominally 2 mm thick and covering a range of carbon contents using a 2 mm reference. The spectra were signal averaged to reduce the noise to an insignificant level. The data were then analysed using the curve fitting program. As the slit width was reduced the apparent carbon content of each sample approached a limiting value. Table 1 summarises the results. The percentage difference between the apparent carbon as measured at  $2\text{ cm}^{-1}$  resolution and at various other slit widths is shown. It may be seen that inadequate resolution leads to large errors in the apparent carbon content at low carbon levels. A resolution of  $5.5\text{ cm}^{-1}$  (corresponding to  $18\mu$  on the PE3000) is adequate to provide good Beers law linearity. This is a much lower resolution than that required by FT machines (reference 2) probably due to the very different instrument functions. The oxygen band is very much broader than the carbon band and it is permissible to use much greater slit width. Generally we use a resolution of about  $7\text{ cm}^{-1}$  ( $18\mu$ ) which is quite adequate to ensure good Beers law linearity. If narrower slit widths are used then interference fringes are observed in the spectra of some samples. In the case of the oxygen absorption measurement both curve fitting and integrated area methods average over several fringes and so these pose no real problem. With the carbon absorption the interference fringes are attenuated by the strong absorption due to the  $610\text{ cm}^{-1}$  band.

### 5.2 Difference in Slit Width Between Sample and Reference

Errors may arise in the apparent carbon content (and to a lesser extent the oxygen content) which are caused by changes in thickness between sample and reference. These may arise both from nonlinearities in the spectrometer and also lack of environmental stability. To assess these errors three samples, nominally 2 mm thick were measured using references of differing thicknesses and also with no reference present. When no reference was used a reference band

attenuator, set to 54% T, was used to provide correction for reflection terms allowed for during conversion of transmittance to absorbance. Results are shown in table 2 which shows very good agreement both between integrated area and curve fitting methods and also insensitivity to thickness mismatch between sample and reference.

### 5.3 Wafer Measurements

Assessment of the curve fitting method for measurements on wafers was carried out using wafers 150  $\mu$ m nominal thickness with resistivities between 10 and 30  $\Omega$ cm cut from known positions in ingots. The actual oxygen and carbon contents of the wafers were estimated by linear interpolation from measurements made on 2 mm samples cut at intervals along the ingots. When making measurements of wafers it was found that under some conditions beats formed between interference fringes in the sample and reference spectra. These beats could cause erroneous results and so for all the measurements on wafers no reference is used. To ensure proper conversion of transmittance to absorbance a reference beam attenuator set to 54% T is used instead of the reference. As before slit width was chosen so as to be a minimum consistent with Beer's law linearity ie to give a resolution of 7  $\text{cm}^{-1}$  for the oxygen band ( 1302 ) and 3.3  $\text{cm}^{-1}$  for carbon.

Table 3 shows results of measurements made using the curve fitting program on 16 wafers with chemically polished both surfaces. The limits over which the curve fitting was made were 1120/1000  $\text{cm}^{-1}$  and 640/300  $\text{cm}^{-1}$ . As discussed below the scan limits may affect the accuracy of the method. Wafer 1 was cut from a region in which the oxygen content in the crystal varied rapidly and so the actual oxygen content is uncertain. The spectra of wafers 11 and 12 showed no obvious reason for their poor performance. As may be seen from the table the measured oxygen contents agree to about 7% with the actual value and the carbon to about  $\pm 1 \times 10^{16}$  atom  $\text{cm}^{-3}$ .

To assess the effects of back surface damage wafers cut adjacent to wafers 11-12 were lapped with #600 emery to produce severe damage. The oxygen and carbon contents were determined using the curve fitting method over the range 1200/1000  $\text{cm}^{-1}$  and 640/300  $\text{cm}^{-1}$ . In all cases the back damaged wafers appeared to contain more oxygen than their chemically etched counterpart (table 4). Changing the algorithm used to convert transmittance to absorbance to correspond with the

assumption that there was no multiple reflection inside the wafer (equation 2.4) gave no significant improvement (table 4). A detailed comparison was made between the fitted spectra and the actual spectra of one of the back damaged wafers. This is shown in figure 2, where it may be seen that systematic errors exist between the fitted and actual spectra. To investigate these errors further a spectrum was created to correspond to the best fit which could be made to the spectrum using the actual oxygen content of the wafer. This is shown in figure 3 compared to the actual spectrum. Also shown in figure 3 is the difference spectrum which represents the residuals. It may be seen that these follow a smooth curve showing that there is curvature of the baseline. To reduce this source of error it was found most convenient to reduce the limits over which the data is fitted to  $1130/1080\text{ cm}^{-1}$ . As shown in table 5 this greatly reduces the systematic errors associated with the back damaged wafers whilst retaining the accuracy of the measurements for the chemically polished wafers.

In table 6 data for wafers have been analysed using both curve fitting and integrated area methods. The integrated area method results used equation 2-4 to convert transmittance to absorbance while the curve fitting method uses equation 2-5. The integrated area measurements for oxygen are systematically 3% low primarily because of the approximation used to convert transmittance to absorbance.

#### 3.4 Heat Treated Samples

When Cz silicon is heat treated precipitates of cristobolite and amorphous  $\text{SiO}_2$  are formed. These precipitates give rise to absorptions at  $1225\text{ cm}^{-1}$ ,  $1120\text{ cm}^{-1}$  and  $1080\text{ cm}^{-1}$  which overlap the  $1106\text{ cm}^{-1}$  interstitial oxygen band. As a result, when measurements of the interstitial oxygen are made using the  $1106\text{ cm}^{-1}$  peak, problems arise in drawing a suitable base line. With the curve fitting method the baseline is fitted using data from all the spectral band being examined. This makes the method much less sensitive to interference from overlapping bands. To test the method a set of 2 mm thick samples with oxygen contents in the range  $1.3 - 1.5 \times 10^{18}\text{ atom cm}^{-3}$  (ASTM F121-76) and carbon contents of  $2-4 \times 10^{16}\text{ atom cm}^{-3}$  (ASTM F123-74) were prepared and isothermally annealed in the range  $650^\circ\text{C} - 1050^\circ\text{C}$ . Figure 4 shows examples of the spectra. In addition to the absorption at  $1106\text{ cm}^{-1}$  interstitial oxygen gives rise to a band at  $515\text{ cm}^{-1}$ . Shimura et al<sup>(3)</sup> have shown that this absorption is due to

unclustered interstitial oxygen. This band suffers very much less from overlap with precipitate bands. It is not often used for quantitative measurement since it is much less intense than the  $1106\text{ cm}^{-1}$  band and its narrow half-width make it unsuitable for wafer measurements where interference fringes would cause severe problems. For well characterised 2mm samples the  $515\text{ cm}^{-1}$  band may be used as a measure of the interstitial oxygen. In figures 5(a) and 6(a) the interstitial oxygen content measured by the peak height at  $1106\text{ cm}^{-1}$  is compared to that determined from the  $515\text{ cm}^{-1}$  band. It may be seen that in the highly precipitated samples the apparent interstitial oxygen content is overestimated by about  $3 \times 10^{17}\text{ atom cm}^{-3}$ . This is due to the underlying precipitate absorptions. When the data were analysed using the curve fitting method in the range  $1130/1080\text{ cm}^{-1}$  (figure 5(b) and 6(b)) very good agreement was found measurement with no sign of systematic error for all anneals below  $1000^{\circ}\text{C}$ . The  $1050^{\circ}\text{C}$  annealed samples showed some sign of systematic error. This is thought to be due to a change in shape of the  $1106\text{ cm}^{-1}$  band due to pairing of the oxygen atoms as distinct from true precipitation. This is discussed more fully by Shimura et al<sup>(3)</sup>.

The results on the heat treated samples show that the curve fitting method is very well suited to making measurements on spectra where the band of interest is superimposed on interfering bands of unknown shape.

## 6 CONCLUSION

Both curve fitting and integrated area measurements may be used to determine the oxygen and carbon content of device quality wafers. It is important to restrict the limits over which the spectra are analysed or systematic errors may be found in back damaged wafers. Instrument resolution is found to affect the accuracy of carbon measurement. The optimum resolution is a compromise between the effects of noise and interference fringes and Beers law non linearity. Although the optimum conditions will vary between instruments the following conditions have been found to give satisfactory results:

Resolution:  $7\text{ cm}^{-1}$  oxygen band  
 $5.5\text{ cm}^{-1}$  carbon band

Curve Fitting method:  $1130 - 1080\text{ cm}^{-1}$  for oxygen  
 $640 - 580\text{ cm}^{-1}$  for carbon

**Integrated Area method:**

Baseline: 1130/1120 and 1090/1080 for oxygen  
: 640/630 and 595/580 for carbon

Peak Area: 1120/1090  $\text{cm}^{-1}$  for oxygen  
630/610  $\text{cm}^{-1}$  for silicon + carbon  
610/595  $\text{cm}^{-1}$  for carbon + silicon

In both cases the scan speed should be chosen to give the desired compromise between accuracy and analysis time.

**ACKNOWLEDGEMENTS**

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TABLE 1  
NON LINEARITIES DUE TO INSTRUMENT RESOLUTION

CARBON AT 2 cm <sup>-1</sup> RESOLUTION	% ERROR AT RESOLUTION SHOWN		
	4 cm <sup>-1</sup>	5.5 cm <sup>-1</sup>	12 cm <sup>-1</sup>
3.5 x 10 <sup>16</sup>	-3	3	43
4.3 x 10 <sup>16</sup>	-5	0	33
5.5 x 10 <sup>16</sup>	0	0	2
8.4 x 10 <sup>16</sup>	5	4	- 9
10.6 x 10 <sup>16</sup>	0	1	7

TABLE 2

## EFFECT OF REFERENCE THICKNESS WITH 2mm NOMINAL THICKNESS SAMPLES

a Integrated Area Method

	Peak	Upper Baseline	Lower Baseline
Oxygen	1125/1090	1180/1145	1065/1030
Silicon + Carbon	626/612	648/632	607/602
Carbon + Silicon	607/602	648/632	607/602

Sample	Oxygen ( $\times 10^{18}$ atom $\text{cm}^{-3}$ )			Carbon ( $\times 10^{16}$ atom $\text{cm}^{-3}$ )			Thickness (mm)		
	Reference Thickness 1.910	2.000	0	Reference Thickness 1.910	2.000	0	Reference Thickness 1.910	2.000	0
#2	1.67	1.67	1.69	3.2	3.6	2.5	1.931	1.939	1.924
#14	1.33	1.32	1.35	5.2	5.4	4.9	1.975	1.985	1.964
#29	.85	.84	.86	13.1	13.2	12.2	1.963	1.971	1.949

b Curve Fitting MethodOxygen band: 1180/1030  $\text{cm}^{-1}$ Carbon band: 640/580  $\text{cm}^{-1}$ 

Sample	Oxygen ( $\times 10^{18}$ atom $\text{cm}^{-3}$ )			Carbon ( $\times 10^{16}$ atom $\text{cm}^{-3}$ )			Thickness (mm)		
	Reference Thickness 1.910	2.000	0	Reference Thickness 1.910	2.000	0	Reference Thickness 1.910	2.000	0
#2	1.67	1.66	1.68	3.4	3.7	2.5	1.931	1.940	1.934
#14	1.33	1.32	1.34	5.2	5.5	5.0	1.977	1.987	1.974
#29	.85	.84	.86	13.2	13.3	12.4	1.965	1.976	1.960

TABLE 3  
CURVE FITTING METHOD ON WAFERS

Scan Limits 1130/1080  $\text{cm}^{-1}$  and 640/580  $\text{cm}^{-1}$  Reference Beam - Attenuator set to 54%. All Wafers Chem Polished.

WAFER	ACTUAL OXYGEN $\times 10^{18}$	MEASURED OXYGEN $\text{atom cm}^{-3}$	ACTUAL CARBON $\times 10^{16}$	MEASURED CARBON $\text{atom cm}^{-3}$	ACTUAL THICKNESS $\mu\text{m}$	MEASURED THICKNESS	TRANSMISSION
A	1.81	1.80	1.4	2.9	360	347	H
B	1.59	1.57	2.1	3.0	338	331	H
C	1.47	1.43	2.8	2.7	364	306	H
D	1.29	1.33	3.9	4.1	364	348	H
E	1.2*	1.12	6.0	6.6	339	328	H
F	1.61	1.55	4.0	4.4	364	370	M
G	1.47	1.49	5.0	5.0	369	357	H
H	1.38	1.10	7.8	6.9	338	361	M
I	1.71	1.65	3.0	2.8	351	338	H
J	1.53	1.43	4.0	2.0	372	409	L
K	1.40	1.31	5.0	4.5	359	349	H
L	1.30	1.27	6.8	7.8	364	353	H
M	1.18	1.19	13.4	9.9	377	371	H
N	1.78	1.68	.4	.4	340	336	H
O	1.57	1.51	.7	1.1	342	332	H
P	1.39	1.40	1.2	1.5	343	339	H
Q	1.20	1.18	1.9	1.8	348	348	H
R	1.10	1.28	3.9	3.9	368	365	H

H = 100% - 50% transmission  
M = 50% - 20% transmission  
L = 20% - 10% transmission  
VL = <10% transmission

TABLE 4

## EFFECT OF BACK SURFACE DAMAGE

SAMPLE	OXYGEN ( $\times 10^{18}$ )		CARBON ( $\times 10^{16}$ )		THICKNESS ( $\mu\text{m}$ )		TRANSMISSION
	ACTUAL	EQN 2.5	EQN 2.4	ACTUAL	EQN 2.5	EQN 2.4	
A	1.81	1.79	1.79	1.4	2.9	2.9	H
A'	1.81	2.01	2.01	1.4	2.4	2.5	VL
B	1.59	1.58	1.61	2.1	3.0	3.0	H
B'	1.59	1.89	1.89	2.1	1.4	1.5	VL
C	1.47	1.44	1.46	2.8	2.7	2.7	H
C'	1.47	1.83	1.82	2.8	2.4	2.4	VL
D	1.29	1.34	1.30	3.9	4.1	4.2	H
D'	1.29	1.59	1.58	3.9	3.8	3.8	L
E	1.2*	1.12	1.11	6.0	6.6	5.6	H
E'	1.2*	1.52	1.52	6.0	5.6	6.6	VL

Wafers A', B', C', D', E' have back surface damage

Scan limits are 1200/1000  $\text{cm}^{-1}$  and 640/580  $\text{cm}^{-1}$

Measurements were made using both equations 2.5 and 2.4 to convert transmittance to absorbance.

TABLE 5

## EFFECT OF SCAN LIMITS ON OXYGEN MEASUREMENT

SAMPLE	ACTUAL OXYGEN	MEASURED OXYGEN	
		1200/1000 $\text{cm}^{-1}$	1130/1080 $\text{cm}^{-1}$
A	$1.81 \times 10^{18}$	$1.79 \times 10^{18}$	$1.80 \times 10^{18}$
A'	$1.81 \times 10^{18}$	$2.01 \times 10^{18}$	$1.79 \times 10^{18}$
B	$1.59 \times 10^{18}$	$1.58 \times 10^{18}$	$1.57 \times 10^{18}$
B'	$1.59 \times 10^{18}$	$1.89 \times 10^{18}$	$1.58 \times 10^{18}$
C	$1.47 \times 10^{18}$	$1.44 \times 10^{18}$	$1.43 \times 10^{18}$
C'	$1.47 \times 10^{18}$	$1.83 \times 10^{18}$	$1.49 \times 10^{18}$
D	$1.29 \times 10^{18}$	$1.34 \times 10^{18}$	$1.33 \times 10^{18}$
D'	$1.29 \times 10^{18}$	$1.59 \times 10^{18}$	$1.39 \times 10^{18}$
E	$1.2 \times 10^{18}$	$1.12 \times 10^{18}$	$1.12 \times 10^{18}$
E'	$1.2 \times 10^{18}$	$1.52 \times 10^{18}$	$1.26 \times 10^{18}$

TABLE 6  
COMPARISON BETWEEN INTEGRATED AREA AND CURVE FITTING METHOD

SAMPLE	OXYGEN ( $\times 10^{18}$ atoms $\text{cm}^{-3}$ ) Integrated Area	OXYGEN ( $\times 10^{18}$ atoms $\text{cm}^{-3}$ ) Curve Fitting	CARBON ( $\times 10^{18}$ atoms $\text{cm}^{-3}$ ) Integrated Area	CARBON ( $\times 10^{18}$ atoms $\text{cm}^{-3}$ ) Curve Fitting	THICKNESS (nm) Integrated Area	THICKNESS (nm) Curve Fitting
A	1.69	1.80	3.8	2.9	376	347
A'	1.69	1.79	4.2	2.4	348	355
B	1.50	1.57	3.4	3.0	367	331
B'	1.47	1.56	2.2	1.4	327	332
C	1.36	1.43	3.1	2.7	340	306
C'	1.38	1.49	1.7	2.4	309	312
D	1.21	1.33	3.9	4.1	370	348
D'	1.31	1.39	4.4	3.8	338	343
E	1.04	1.12	7.1	6.6	396	328
E'	1.21	1.26	7.6	5.6	317	321

Integrated area limits: Baseline 1130/1120; 1070/1060 and 640/630; 595/580

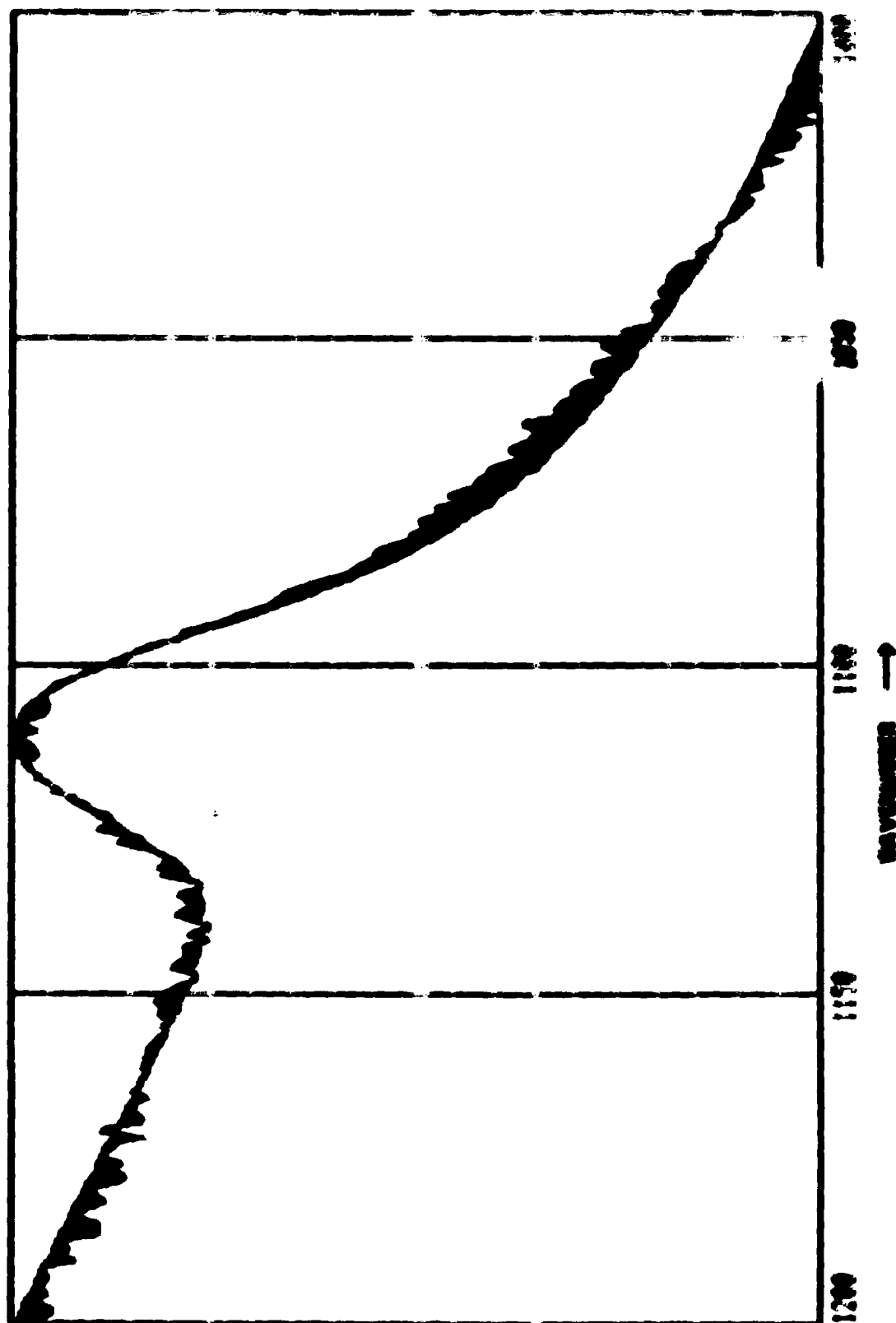
Oxygen Peak 1120/1070  $\text{cm}^{-1}$

Silicon Peak 630/ 610  $\text{cm}^{-1}$

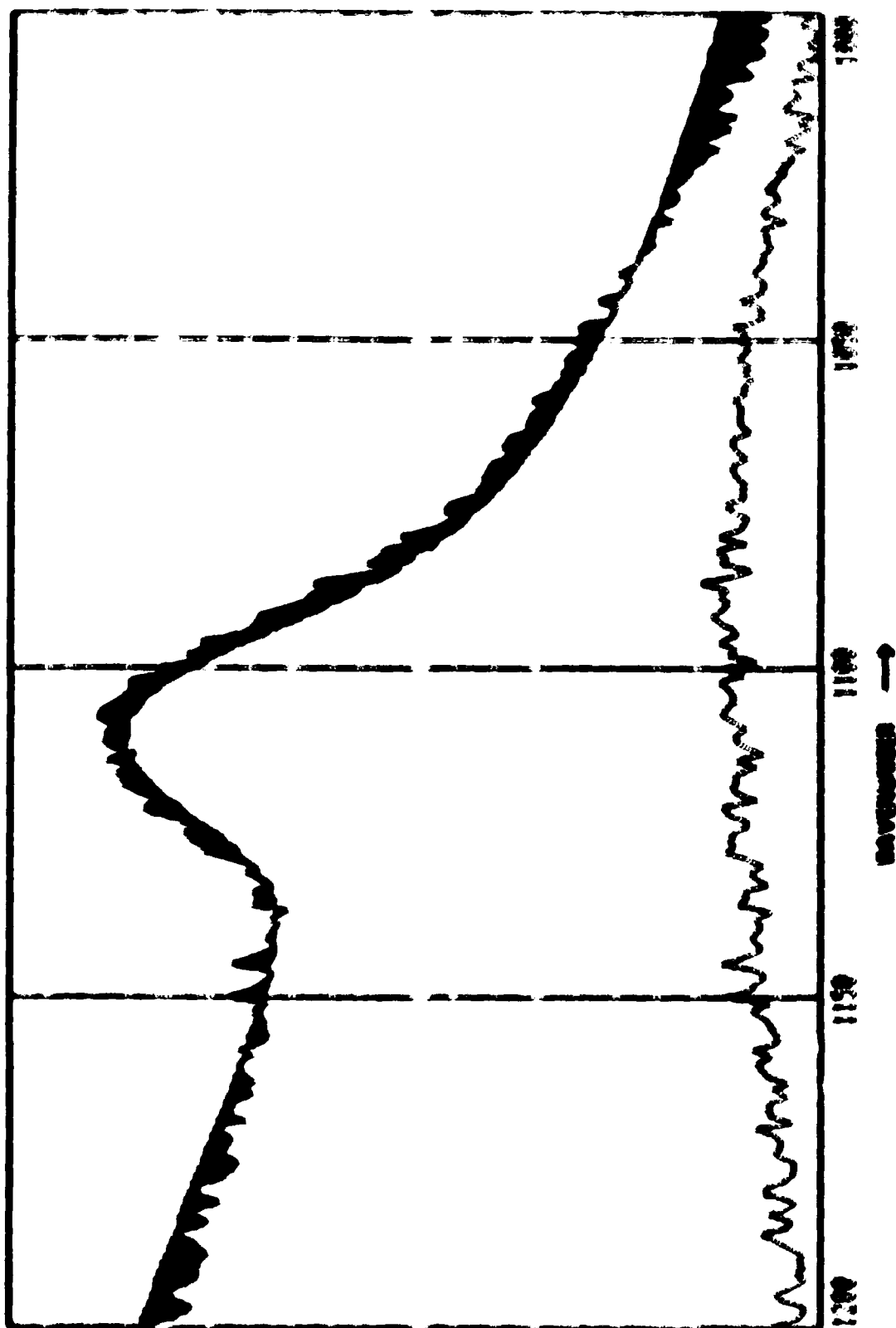
Carbon Peak 610/ 595  $\text{cm}^{-1}$

Curve fitting method limits: 1130/1060 and 640/580  $\text{cm}^{-1}$

The integrated area method uses equation 2.4 to convert transmittance to absorbance and the curve fitting method equation 2.5.

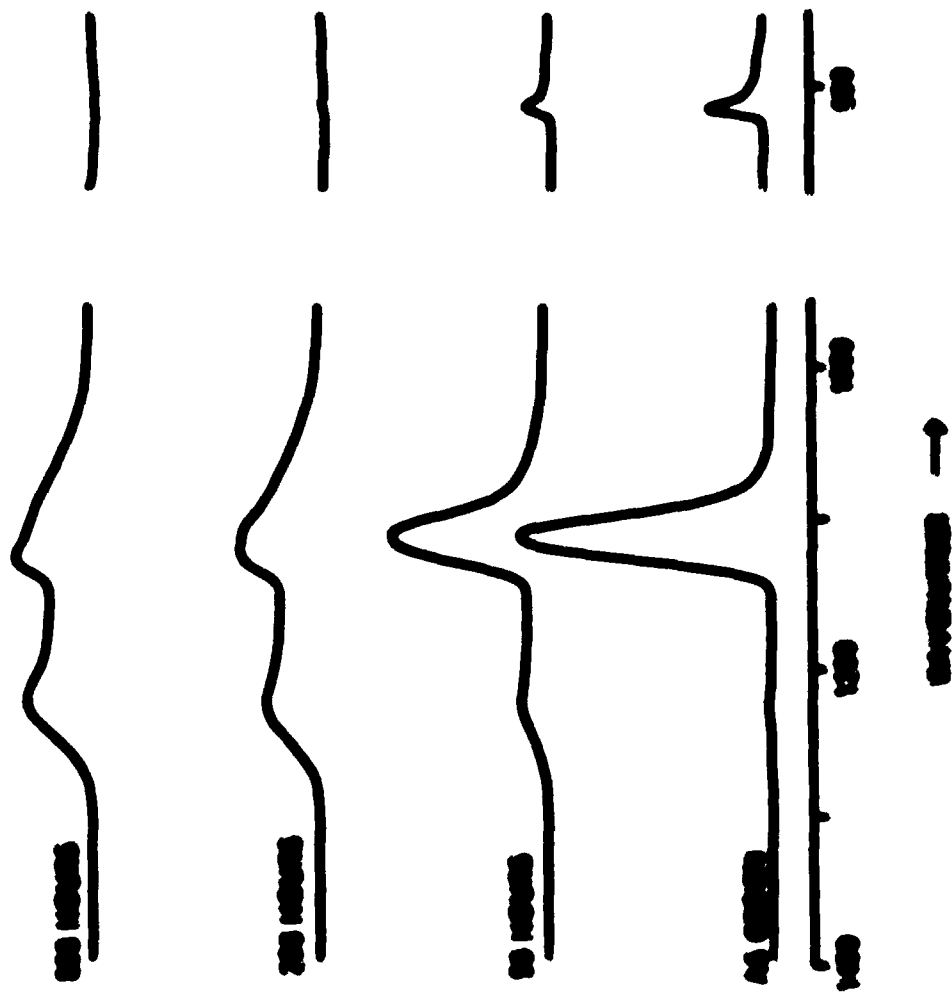


**FIGURE 2** Measured spectra for water D' compared to best fit curve.  
The difference between the two curves is shaded.



**FIGURE 3** Measured spectra for water D' compared to spectrum calculated from actual oxygen content. (The difference between the two spectra is shaded.) Lower curve shows difference spectra which represents residuals.





0.1A spectra of C<sub>60</sub> molecule  
 showing the chemical shift  
 of the molecule

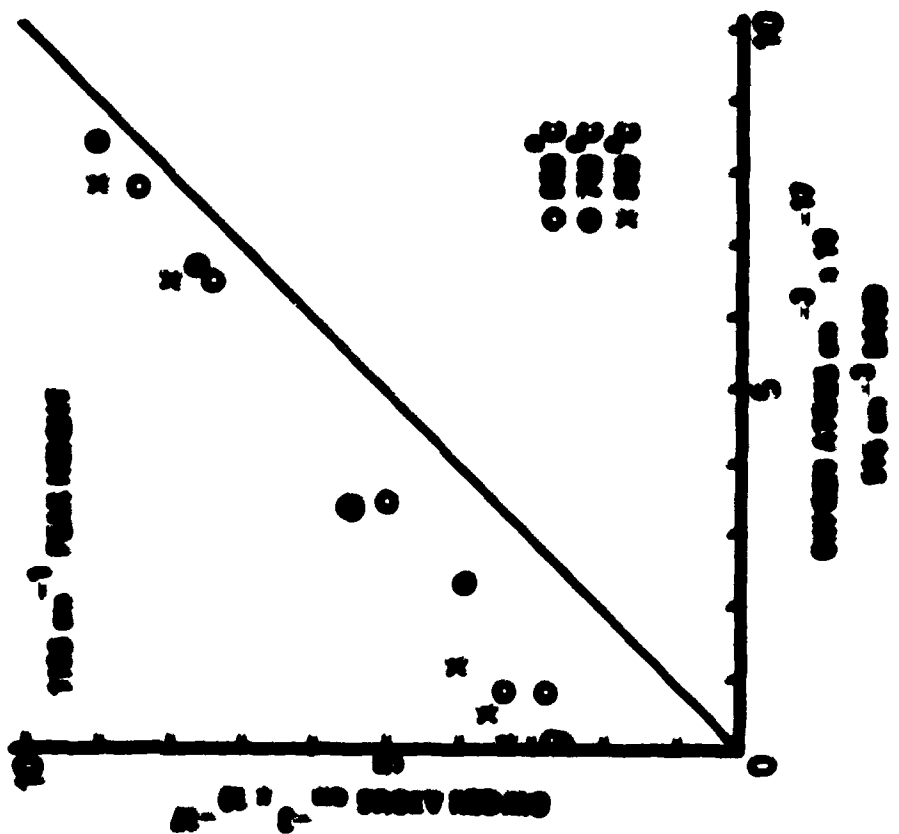
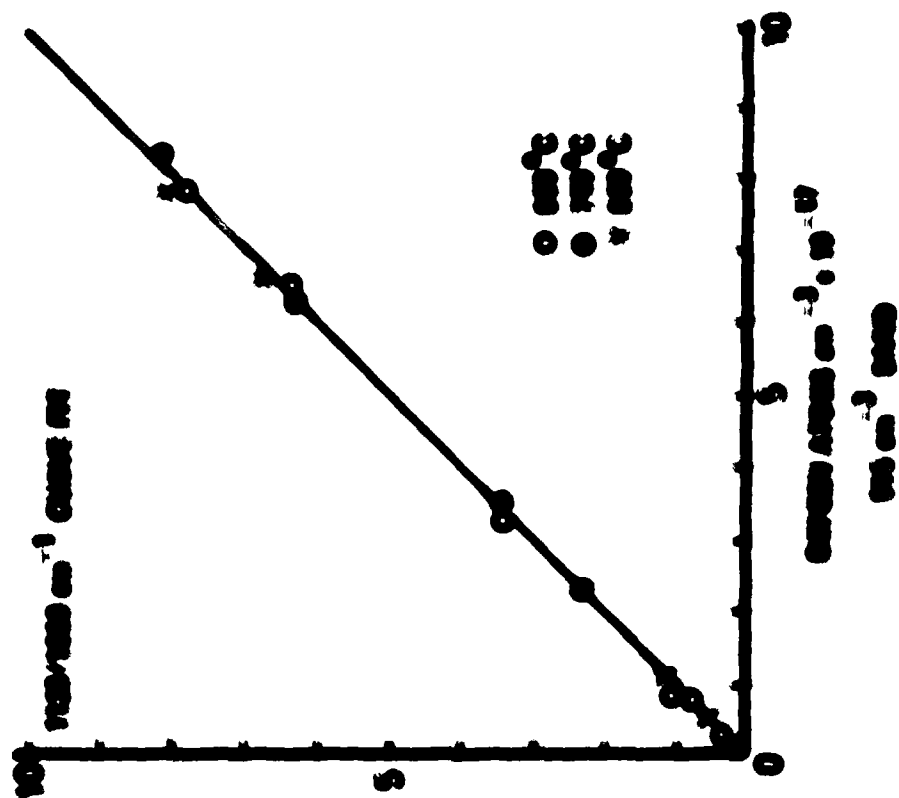


Figure 1. Change in the 1720-1820  $\text{cm}^{-1}$  band with temperature for the 100°C, 150°C, and 200°C isotherms. The 100°C isotherm is the only one which shows a significant change in the 1720-1820  $\text{cm}^{-1}$  band with temperature.

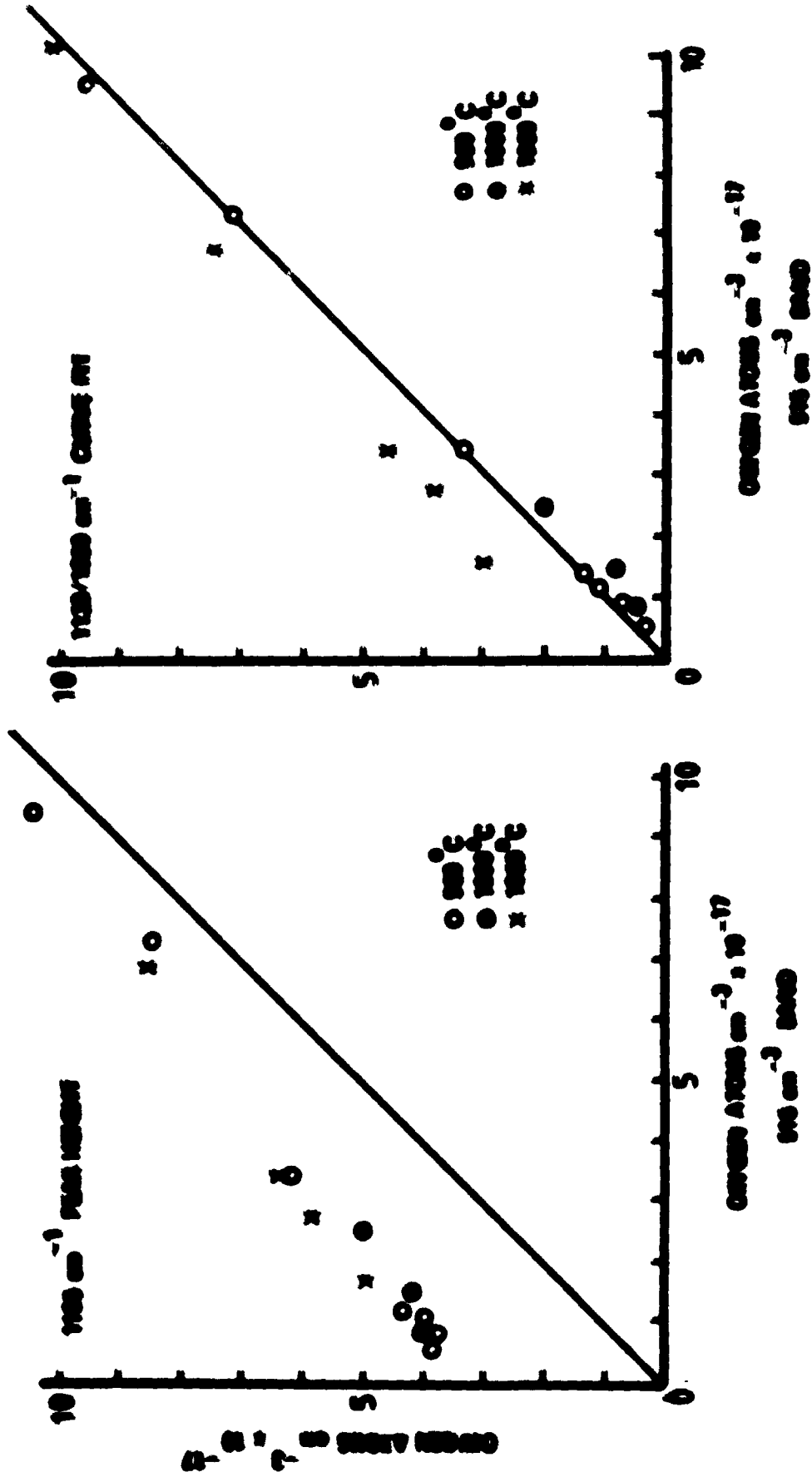


FIGURE 1. Integrated absorption of  $\text{SiH}_4$  as a function of concentration. The data were obtained from the following sources: (a) 1700  $\text{cm}^{-1}$  peak height in 1700/1680  $\text{cm}^{-1}$  ratio; (b) 1720/1680  $\text{cm}^{-1}$  contour area. The data were obtained from the following sources: (a) 1700  $\text{cm}^{-1}$  peak height in 1700/1680  $\text{cm}^{-1}$  ratio; (b) 1720/1680  $\text{cm}^{-1}$  contour area. The data were obtained from the following sources: (a) 1700  $\text{cm}^{-1}$  peak height in 1700/1680  $\text{cm}^{-1}$  ratio; (b) 1720/1680  $\text{cm}^{-1}$  contour area.

